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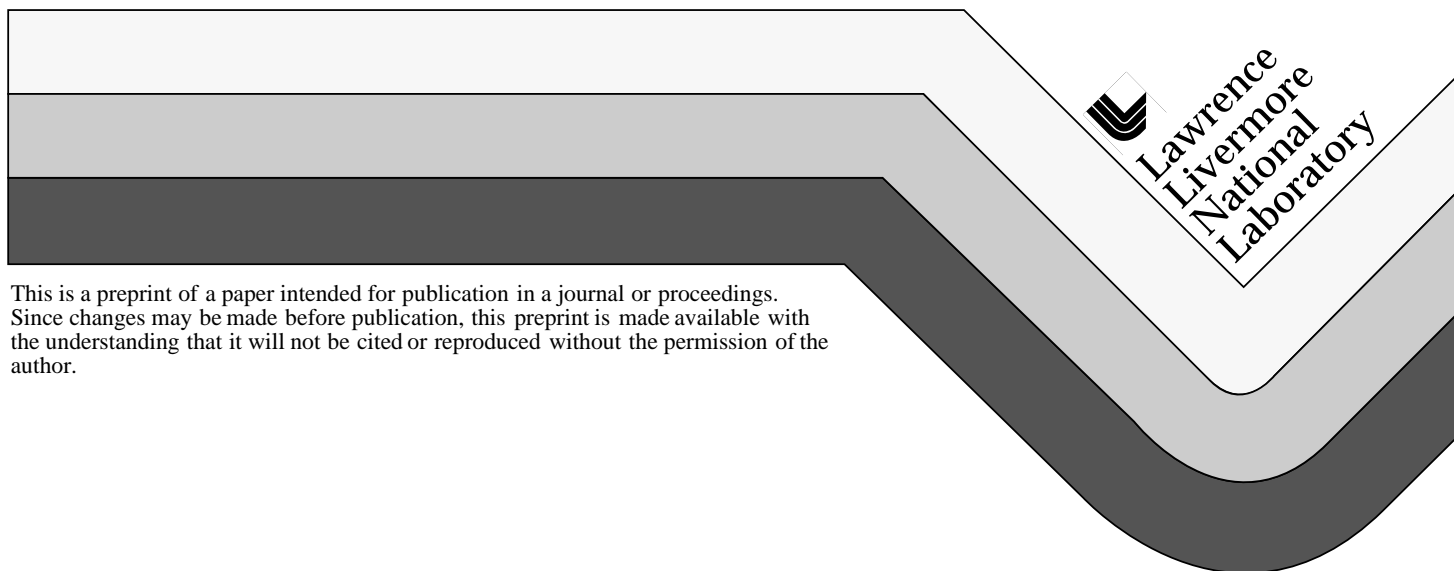
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Thermostatics and Thermokinetics of Closed Combustion Systems

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Abstract

The paper presents a formalism for defining the intrinsically non-linear behavior of a closed combustion system in terms especially suited for its control. Its implementation is illustrated by application to a diesel engine.

Thermostatics

Thermostatics provides an account of energy transformation taking place in a closed combustion system, based on the energy balance supported by the balances of mass and volume. Yielded thereby are profiles of the mass averaged thermodynamic parameters of all the components: air, fuel, as well as charge, reactants and products with respect to pressure and of time. In particular, a relationship is thus established between the fraction of consumed fuel – the input to a closed system – and the generated pressure – its intrinsic output.

The literature on this subject is very rich, indeed, as expected of a topic bearing incisively upon the automobile and oil industries, a conglomerate occupying today one of the largest economic sectors in the world. This is manifested in all the textbooks on piston engines, as well as in all the classical monographs on combustion, let alone the plethora of papers published throughout the world.

Parameters

In terms of conventional symbols, adopted here as the principal thermodynamic reference parameter is

$$\mathbf{w}_K \equiv \mathbf{p}_K \mathbf{v}_K \quad (1)$$

where $K = A, F, C, R, P$ and S , refer, respectively, to the components: fuel, air, charge, reactants, products and to the system. The thermodynamic pressure (i.e. the thermodynamic parameter of state, rather than the aerodynamic variable in the equation of motion) is considered as spatially uniform. Hence

$$\mathbf{p}_K = \mathbf{p}(\mathbf{t}) \quad (2)$$

where \mathbf{t} , the time, is the primary independent variable, which, for piston engines, is expressed by the crank angle, $\Theta \propto \mathbf{t}$. (For clarity, we adopt the convention that variables are represented as bold block letters, while their associated constant values appear as normal block letters).

The thermodynamic properties of the components are expressed most conveniently in terms of the Le Chatelier diagram - a plot of the loci of their states on the plane of internal energy, \mathbf{u} , as a function of \mathbf{w} , defined by (1). Noting that the loci of states of the components are, within the regimes of their applicability, practically linear, they are expressed by straight lines, as shown in Fig. 1. All the coordinates are normalized then with respect to the initial state of the air, A_i , so that $W_{Ai} = U_{Ai} = 1$. Thus, the normalized pressure and specific volume are $\mathbf{P} \equiv \mathbf{p}/p_i$ and $\mathbf{v} \equiv \mathbf{v}/v_i$ while the thermodynamic reference parameters and internal energies are expressed as

$$\mathbf{W}_K \equiv \frac{\mathbf{w}_K}{w_{Ai}} \quad (3)$$

and

$$\mathbf{U}_K \equiv \frac{\mathbf{u}_K - u_{K0}}{C_A w_{Ai}} = k_K \mathbf{W}_K - Q_K \quad (4)$$

where $C_K \equiv d\mathbf{u}_K/d\mathbf{w}_K = \Delta \mathbf{u}_K / \Delta \mathbf{w}_K$, $k_K \equiv C_K/C_A$, while, in terms of $u_{K0} \equiv \mathbf{u} @ \mathbf{w} = 0$,

$$Q_K = \frac{(u_{A0} - u_{K0})}{C_A w_{Ai}} \quad (5)$$

so that $k_A = 1$ and $Q_A = 0$. Upon the recognition that, except for products, the relationship between pressure and specific volume of all the components is, in effect, polytropic,

$$W_K = W_{Ki} P^{1-1/n_K} \quad (6)$$

for which $W_{Ki} \equiv w_{Ki}/w_{Ai}$. Finally, the energy expenditure is expressed as

$$U_E = \omega + \kappa \quad (7)$$

where $\omega \equiv \int P dv_S / C_A$ is the work performed by the system, while $\kappa \equiv q_w / C_A w_{Ai}$ expresses the energy lost by heat transfer to the walls.

Balances

The **mass balance** is expressed in terms of the mass fractions of the intrinsic components Y_K ($K = A, F, P$). The mass fraction of the products, Y_P , is adopted as the progress parameter. Thus, at the initial state of $Y = 0$, marked by subscript i , the mass fraction of fuel in the charge is $Y_{Fi} = F_C$, while at the final state, denoted by f , $Y_{Ff} = 0$. Concomitantly the mass fraction in products of fuel consumed for their generation is F_R .

The intensive thermodynamic properties: w , defined by (1) and u , the internal energy, are transformed into $Z_K = W_K$ or U_K ($K = C, R$) by turbulent mixing so that

$$Z_K = Z_A + (Z_F - Z_A) \quad (8)$$

whence,

$$Z_F Y_F + Z_A Y_A = Z_C - Z_R Y \quad (9)$$

The **volume** and **energy balances** can be expressed then comprehensively in terms of Z as follows:

$$Z_F Y_F + Z_A Y_A + Z_P Y_P = Z_C + (Z_P - Z_R) Y = Z_S \quad (10)$$

In terms of the normalized parameters specified by (3-7) one obtains finally the following expression for the mass fraction of products

$$x_F = \frac{F_R}{F_C} \frac{a P v_S - b P^{1-1/n_c} - c + \omega + \kappa}{\Delta Q - d P^{1-1/n_c}} \quad (11)$$

where $a \equiv k_P W_{Ci}$, $b \equiv (k_P - k_C) W_{Ci}$, $c \equiv k_C W_{Ci}$, $d \equiv (k_P - k_R) W_{Ri}$ and $\Delta Q \equiv (Q_P - Q_R)$.

Energy Loss

The mass fraction of fuel expended by heat loss to the walls, κ , is evaluated on the basis of a correlation developed on the basis of extensive research on heat transfer from combustion in enclosures of constant volume. Towards this end, the mass fraction of fuel consumed by combustion, expressed by (11) is expressed simply as

$$x_F = x_p + x_q \quad (12)$$

Subscript “p” denoting its effective part, specified by (11) with $\kappa = 0$, while “q” refers to the ineffective rest. As displayed on Fig. 4, the correlation we deduced from an extensive experimental study carried out under the direction of Greif and Oppenheim is expressed in terms of the following power law

$$x_{pn} \equiv \frac{x_p}{x_{pf}} = 1 - (1 - x_F)^\sigma \quad (13)$$

wherefore, according to experimental data,

$$\sigma = 2 - x_{pf}^{3/2} \quad (14)$$

The numerator of (13) is evaluated from (11), for $\kappa = 0$, while the denominator $x_{pf} = x_{pmax}$. Thus, x_{pn} is expressed as an explicit function of P and v_S . The total mass fraction of fuel consumed by the exothermic

process of combustion is then in terms of the following correlation

$$\mathbf{x}_F = 1 - (1 - \mathbf{x}_{pn})^{1/\sigma} \quad (15)$$

Thermokinetics

Thermokinetics considers the behavior of a closed combustion system in terms akin to kinematics of motion. Traditionally, the mass rate of reactants consumed by combustion is expressed in combustion literature as

$$\frac{d\mathbf{M}_b}{dt} = \rho_u \int_{A_{flame}} \mathbf{S}_u d\mathbf{A} \quad (16)$$

where \mathbf{M}_b is the burned mass, ρ_u - the density of the unburned substance, \mathbf{S}_u - the so-called normal burning speed and \mathbf{A} - the frontal area. This expression has been of key significance in the development of laminar flame theory. It is correct, however, only as long as the geometry of the front is plane, line, or point symmetrical. In the case of wrinkled fronts, it becomes problematic because of the dependence of \mathbf{S}_u on the curvature of the front, while in a turbulent field it loses its entire meaning because the front is then a fractal, causing it to become dimensionally inconsistent. Instead then we adopt for this purpose a global expression of the form of

$$\frac{d\mathbf{X}_k}{dt} = \frac{\mathbf{X}_{kf}}{T} \mathbf{x}_k(\mathbf{x}, \tau) \quad (17)$$

where $\tau \equiv \frac{t}{T}$ and $\mathbf{x}_k \equiv \frac{\mathbf{X}_k}{\mathbf{X}_{kf}}$, while $T \equiv t_f - t_i$, is the life time, and $\mathbf{X}_k = \mathbf{M}_b, \mathbf{M}_F, \Pi$ ($k = \beta, F, \Pi$), where the latter is defined as

$$\Pi \equiv \mathbf{P}v^{n_e} - 1 \quad (18)$$

Formulation

The kinetic behavior of the exothermic process of combustion is expressed then in terms of a modified exponential yielded by the following conditions of growth

$$\frac{d\mathbf{x}}{d\tau} = \lambda(\xi + \mathbf{x})(1 - \tau)^\chi \quad (\chi > 0) \quad (19)$$

so that @ i: $d\mathbf{x}/d\tau = \lambda\xi > 0$, while @ f: $d\mathbf{x}/d\tau = 0$.

Life Function

The integral of (19) yields an expression for the trajectory of $\mathbf{x}(\tau)$ in form of a time modulated exponential growth we call the life function

$$\mathbf{x} = \frac{e^\xi - 1}{e^{\xi_f} - 1} \quad (20)$$

wherefore

$$\xi = \frac{\lambda}{\chi + 1} [1 - (1 - \tau)^{\chi + 1}] \quad (21)$$

Implementation

The implementation of the analysis is illustrated here by application to a Caterpillar C12 diesel engine. Its power was 245 kW, Speed: 1200 rpm, Torque: 82 Nm, BMEP: 2.04 MPa, fuel flow rate: 880 g/min, air/fuel ratio: 22.77 ($\lambda = 1.6$). A sample of results is displayed in Figs. 2-8.

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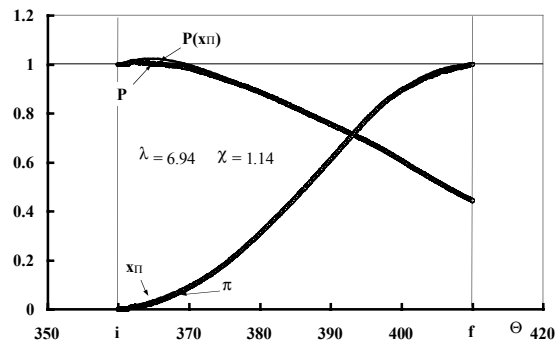


Fig. 3. Measured Pressure and its Analytic Expression

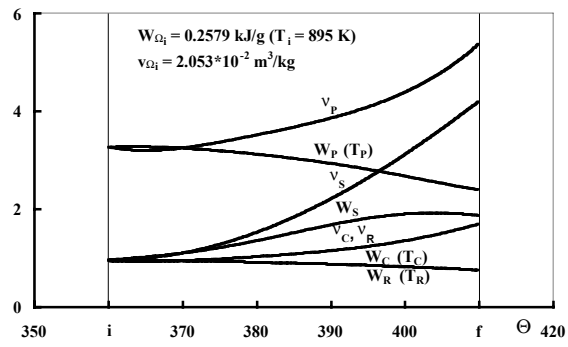


Fig. 4. Thermodynamic Parameters

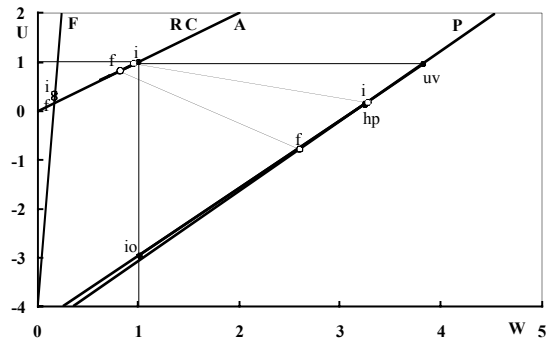


Fig. 5. Le Chatelier Diagram

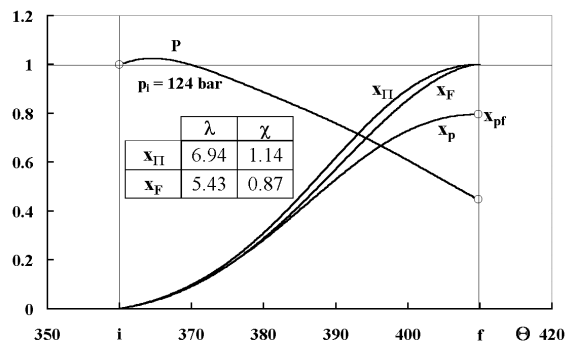


Fig. 6. Life Functions

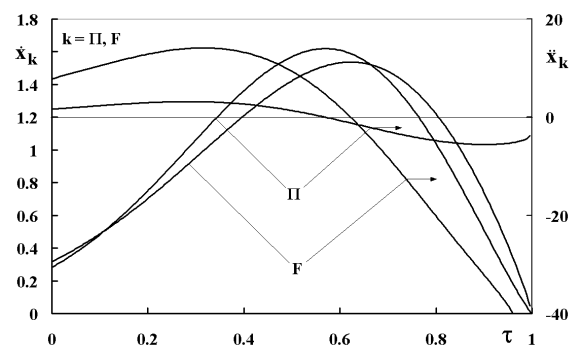


Fig. 7. Thermokinetic Parameters

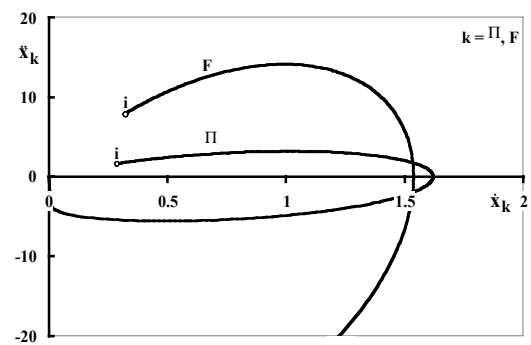


Fig. 8. Thermokinetic Polar Diagram